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Factorization of Simulations

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Abstract

A simulation is collection of agents that, according to some schedule, are making decisions based on information about other agents in that collection. In this paper we present a class of dynamical systems called Sequential Dynamical Systems (SDS) that was developed to capture these key features of computer simulations. Here, as an example of the use of SDS, we demonstrate how one can obtain information about a simulation by a factorization into smaller simulations.

1. Introduction.

In a simulation, be it a traffic study, a packet routing problem or a stock market analysis, one can usually identify the following components: A collection of agents/atoms/entities, decision or update rules for each agent and a scheduling mechanism. Typically, the update rule of an agent only depends on the state of the agents in its vicinity, and thus we speak about *local* rules. Simulations can be viewed as the generation of global dynamics from local dynamics caused by agent interaction, i.e., composition of local rules.

Sequential Dynamical Systems, or SDS for short, were constructed as a mathematical abstraction of the above. Specifically, agents are interpreted as the vertices in a graph, and two vertices are connected if the corresponding agents can communicate. Associated to each vertex in the graph there is a state and also a function that depends on the neighbor states in the graph. The latter corresponds to the decision rule of an agent. Finally, the update mechanism is implemented as a permutation. The dynamics of SDS results from applying the local functions in the order given by the permutation and then by iterating this. For the construction of SDS and the subsequent studies of their properties we refer to [1, 2, 3, 4, 5, 6, 7, 8]. Lately, SDS has also been studied from a computational/complexity point of view. In fact, an SDS can be viewed as an algorithm, and under quite general conditions it can be shown that all equivalent algorithms have a complexity at least that of the SDS-algorithm. For the computational complexity approach we refer to [9]

In the remainder of the introduction we will briefly go through the necessary prerequisites and the definition of SDS. We will then give some very recent results on SDS that shows how it is possible to factorize a simulation (SDS) and from these simpler factors obtain information about the dynamics of the original simulation (SDS). This is clearly related to the question of constructing/implementing computationally efficient simulations. The theoretical results will be illustrated by simple examples.

Let Y be a labeled graph with vertex-set $\mathbf{v}[Y] = \mathbb{N}_n = \{1,2,3,\ldots,n\}$, which we write as $Y < K_n$. The edge-set of Y is denoted by $\mathbf{e}[Y]$. Let $S_{1,Y}(i)$ be the set of Y-vertices that are adjacent to vertex i, let $\delta_i = |S_{1,Y}(i)|$ and let $d = \max_{i \in \mathbb{N}_n} \delta_i$. The increasing sequence of elements of $S_{1,Y}(i)$ with i prepended is denoted by

$$\tilde{B}_{1,Y}(i) = (i, j_1, \dots, j_{\delta_i}).$$
 (1)

To each vertex i we associate a state $x_i \in \mathbb{F}_2$, and we write $x = (x_1, x_2, \dots, x_n)$ for the system state. For each $k = 1, \dots, d+1$ we have a function f, that for simplicity we assume to be symmetric, and for each vertex i we introduce a map

$$\operatorname{proj}_{Y[i]} : \mathbb{F}_2^n \to \mathbb{F}_2^{\delta_i + 1},$$

$$(x_1, \dots, x_n) \mapsto (x_i, x_{j_1}, \dots, x_{j_{\delta_i}}).$$

$$(2)$$

The map projects from the full n-tuple x down to the states vertex i needs for updating its state. For each $i \in \mathbb{N}_n$ there is a Y-local map $F_{i,Y} : \mathbb{F}_2^n \to \mathbb{F}_2^n$ given by

$$y_i = f_{\delta_i+1} \circ \text{proj}_Y[i],$$

 $F_{i,Y}(x) = (x_1, \dots, x_{i-1}, y_i(x), x_{i+1}, \dots, x_n).$ (3)

The function $F_{i,Y}$ updates the state of vertex i and leaves all other states fixed. We refer to the sequence $(F_{i,Y})_i$ as F_Y . Note that for each graph $Y < K_n$ a sequence $(f_k)_{1 \le k \le n}$ induces a sequence F_Y , i.e. we have a map $\{Y < K_n\} \to \{F_Y\}$. We define the map $[F_Y,]: S_n \to \operatorname{Map}(\mathbb{F}_2^n, \mathbb{F}_2^n)$ by

$$[F_Y, \pi] = \prod_{i=1}^n F_{\pi(i), Y}, \tag{4}$$

where product denotes ordinary function composition.

Definition 1 (Sequential Dynamical System) Let $Y < K_n$, let $(f_k)_k$ with $1 \le k \le d(Y) + 1$ be a sequence of symmetric functions as above, and let $\pi \in S_n$ The sequential dynamical system (SDS) over Y induced by $(f_k)_k$ with respect to the ordering π is $[F_Y, \pi]$.

Example 1 Let $Y = \text{Circ}_4$ as shown in figure 1. With the parity function, i.e. $\text{par}_3 : \mathbb{F}_2^3 \to \mathbb{F}_2$ de-



Figure 1. The circle graph on 4 vertices, Circ₄.

fined by $\operatorname{par}_3(x_1, x_2, x_3) = \sum_i x_i \mod 2$, update order (1, 2, 3, 4) and initial state (1, 1, 0, 0) we get

$$\begin{aligned} \operatorname{Par}_1(1,1,0,0) &= (0,1,0,0), \\ \operatorname{Par}_2 \circ \operatorname{Par}_1(1,1,0,0) &= (0,1,0,0), \\ \operatorname{Par}_3 \circ \operatorname{Par}_2 \circ \operatorname{Par}_1(1,1,0,0) &= (0,1,1,0), \\ \operatorname{Par}_4 \circ \operatorname{Par}_3 \circ \operatorname{Par}_2 \circ \operatorname{Par}_1(1,1,0,0) &= (0,1,1,1), \end{aligned}$$

and thus
$$[\mathbf{Par}_{Circ_4}, (1, 2, 3, 4)](1, 1, 0, 0) = (0, 1, 1, 1).$$

Since phase space for an SDS is finite we may identify it with a finite unicyclic digraph.

Definition 2 The digraph $\Gamma[F_Y, \pi]$ associated to the SDS $[F_Y, \pi]$ is the directed graph having vertex-set \mathbb{F}_2^n and directed edges $\{(x, [F_Y, \pi](x)) \mid x \in \mathbb{F}_2^n\}$.

Note that the choice of $\mathbb{F}_2 = \{0,1\}$ for the state values could be changed to any finite field with only minor modifications. In fact, some results obtained on SDS does not even require finiteness - one could pick, e.g. real values.

2. Factorization of SDS

To begin, recall that a morphism between graphs Y and Y' is a pair $\phi = (\phi_1, \phi_2)$ with $\phi_1 : v[Y] \to v[Y']$ and $\phi : e[Y] \to e[Y']$ such that

$$\forall e = \{i, j\} \in e[Y] : \phi_2(e) = \{\phi_1(i), \phi_1(j)\}.$$

In other words, adjacent vertices in Y are mapped to i) adjacent vertices in Y' or ii) to the same vertex in Y'. A morphism of directed graphs also preserves the direction of edges.

A graph morphism $\phi: Y \to Y'$ is *locally bijective* if

$$\forall i \in v[Y] : \phi|_{B_{1,Y}(i)} : B_{1,Y}(i) \to B_{1,Y'}(\phi(i))$$

is bijective. Note that locally bijective does not imply bijective as the following example shows.

Example 2 A locally bijective graph morphism $\phi: Q_2^3 \to K_4$, see figure 2. The map ϕ_1 is defined by $\phi_1(\{0,7\}) = \{1\}$, $\phi_1(\{1,6\}) = \{2\}$, $\phi_1(\{2,5\}) = \{3\}$, $\phi_1(\{3,4\}) = \{4\}$, and ϕ_2 is the induced edge-map. The resulting graph morphism is clearly locally bijective, but not bijective.

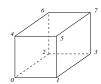




Figure 2. The graphs Q_2^3 and K_4 .

Definition 3 Let $[F_Z, \sigma]$ and $[F_Y, \pi]$ be two SDS. An SDS-morphism between $[F_Z, \sigma]$ and $[F_Y, \pi]$ is a pair (ϕ, Φ) where $\phi: Y \to Z$ is a graph morphism and where $\Phi: \Gamma[F_Z, \sigma] \to \Gamma[F_Y, \pi]$ is digraph morphism.

Given a graph morphism $\phi: Y \to Z$ we want to relate the dynamics of SDS over the two graphs Y and Z. In most cases here the local functions will be the same. To begin, we relate update schedules over Y and Z via ϕ . Assume $|\mathbf{v}[Y]| = n$ and $|\mathbf{v}[Z]| = m$ and let $\phi^{-1}(i) = \{i_1, \ldots, i_{l_i}\}$ where $i_1 < \ldots i_{l_i}$ for $1 \le i \le m$. Define the map $\eta_\phi: S_m \to S_n$ by

$$\eta_{\phi}(\pi = (\pi_1, \pi_2, \dots, \pi_m)) \\
= (\pi_{11}, \dots, \pi_{1l_{\pi_1}}, \dots, \pi_{m1}, \dots, \pi_{1l_{\pi_m}}).$$
(5)

For instance, in the example with $\phi: Q_2^3 \to K_4$, we have $\eta_{\phi}(4,3,2,1) = (3,4,2,5,1,6,0,7)$. Finally, we define the map $\tau: \mathbb{F}_2^m \to \mathbb{F}_2^n$ by $(\tau(x))_k = x_{\phi(k)}$. The dynamics of SDS over Y and Z can now be related in the following way [8]:

Theorem 1 Let Y and Z be loop-free connected graphs, and let $\phi: Y \to Z$ be a bijective graph morphism. Suppose the same sequence $(f_i)_i$ of Boolean quasi-symmetric local functions is used for both graphs. Then the map τ induces a natural embedding

$$T: \Gamma[F_Z, \pi] \hookrightarrow \Gamma[F_Y, \eta_\phi(\pi)]. \tag{6}$$

Proof. Here we will only outline the ideas of the proof. The full detail may be found in [8]. First, since ϕ is local bijection the set $\phi^{-1}(i) = \{j_1, \ldots, j_{l_i}\}$ is an independence set of Y for all $i \in \mathbf{v}[Z]$. Thus we may compose the functions F_k , $k \in \phi^{-1}(i)$ in any order we like, e.g. increasing index order. Now, careful inspection yields

$$\prod_{j=1}^{m} \left[\prod_{d \in \phi^{-1}(i_j)} F_{Y,d} \right] \circ \tau = \tau \circ \prod_{j=1}^{m} F_{Z,i_j}, \tag{7}$$

which in turn means $[F_Y, \eta_{\phi}(\pi)] \circ \tau = \tau \circ [F_Z, \pi]$.

Example 3 To illustrate the use of Theorem 1 we show how to relate the phase space of $[\mathbf{Min}_{K_4}, \mathrm{id}_4]$ to that of $[\mathbf{Min}_{Q_2^3}, (0,7,1,6,2,5,3,4)]$. Here \mathbf{Min}_Y denotes the sequence of local functions induced by the minority functions $\min: \mathbb{F}_2^k \to \mathbb{F}_2$ which return 1 if the number of

1's is strictly less than the number of 0's, and 0 otherwise. From the example above we have the bijective graph morphism $\phi: Q_2^3 \longrightarrow K_4$. Next note that $\eta_{\phi}(\mathrm{id}_4) = (0,7,1,6,2,5,3,4)$. We know that $[\mathbf{Min}_{K_4},\mathrm{id}_4]$ has exactly two 5-cycles and no fixed points. The two 5-cycles are shown in the top row of figure 3. For convenience we use the map

$$\xi_i : \mathbb{F}_2^i \longrightarrow \mathbb{N}, \qquad \xi_i(x_1, \dots, x_i) = \sum_{j=0}^i x_j \cdot 2^{j-1} \quad (8)$$

to encode states (binary tuples), and we have, e.g. $(1,1,0,1) \mapsto 1+2+8=11$. It is straightforward to see that the phase space of $[\mathbf{Min}_{K_4}, \mathrm{id}_4]$ is indeed embedded in the phase space of $[\mathbf{Min}_{Q_3^3}, (0,7,1,6,2,5,3,4)]$.

We remark that $[\mathbf{Min}_{Q_2^3}, \eta_\phi(\mathrm{id}_4)]$ has two fixed points in addition to the two 5-cycles shown in the last row in figure 3. These fixed points are related by the graph automorphism $\gamma = (07)(16)(25)(34)$, and consequently, so are their transients. Stated differently, the two components in $\Gamma[\mathbf{Min}_{Q_2^3}, \eta_\phi(\mathrm{id}_4)]$ containing the fixed points are isomorphic. Their structure is shown in figure 4.

The following result links the existence of certain subgroups of \mathbb{F}_2^n to the existence of covering maps of the *n*-cube.

Theorem 2 For any subgroup $H' < \mathbb{F}_2^n$ with $[\mathbb{F}_2^n : H'] \ge n+1$ there exists an isomorphic subgroup H H' that has the property $H(x) \cap H(y) = \emptyset$ for $x \ne y$; $x,y \in \{0,e_1,\ldots,e_n\}$.

For each subgroup $H < \mathbb{F}_2^n$ with the property $H(x) \cap H(y) = \emptyset$ for $x \neq y$; $x,y \in \{0,e_1,\ldots,e_n\}$ the graph $H \setminus Q_2^n$ is connected, undirected and loop-free and the natural projection

$$\pi_H: Q_2^n \longrightarrow H \setminus Q_2^n, \quad v \mapsto H(i)$$

is a covering-map.

For the proof we refer to [5]. In particular we have the following result [8] for *n*-cubes:

Proposition 1 There exists a locally bijective graph morphism

$$\phi: Q_2^n \longrightarrow K_{n+1} \tag{9}$$

if and only if $2^n \equiv 0 \mod n + 1$ holds.

Thus, whenever n+1 divides 2^n we can obtain information about SDS over the n-cube from that of the SDS over the complete graph on n+1 vertices. The analysis of systems over the complete graph is generally a lot simpler than what one will find for other graphs. Moreover, we note that an SDS over the n-cube has 2^{2^n} states while an SDS over K_{n+1} has 2^{n+1} states [8]. The fact that systems over the complete graph tend to be simpler to understand can be used in the following way:

Proposition 2 Assume $2^n \equiv 0 \mod n + 1$, and let $\pi \in S_{n+1}$. Then there exists a covering $\phi: Q_2^n \to K_{n+1}$ and the SDS $[\mathbf{Par}_{Q_2^n}, \eta_{\phi}(\pi)]$ has a periodic orbit of length n + 2

Proof. We will establish the existence of the covering map $\phi: Q_2^n \to K_{n+1}$ under the above condition in the next section. Since a covering map is locally bijective, we deduce that the phase space of $\Phi = [\mathbf{Par}_{K_n}, \pi]$ can be embedded into the phase space of $\Psi = [\mathbf{Par}_{Q_2^n}, \eta_{\phi}(\pi)]$. Thus we see that whatever we can deduce about the smaller system Φ applies to the larger system Ψ . The phase space of Ψ has 2^{2^n} points while that of Φ has 2^{n+1} points.

One particular consequence of this is that every periodic orbit for Φ will also be a periodic orbit for Ψ . We will show that Φ always have a periodic orbit of length n+2. For simplicity we take $\pi=\mathrm{id}_{n+1}$.

By inspection $\operatorname{Par}_n:\mathbb{F}_2^n\to\mathbb{F}_2^n$ is seen to satisfy the functional relation

$$\psi(x_1, \dots, x_{n-1}, \psi(x_1, \dots, x_n)) = x_n.$$
 (10)

As a consequence of this we derive

$$x = (x_1, x_2, \dots, x_n)$$

$$\stackrel{1}{\rightarrow} (\operatorname{Par}_n(x), x_2, x_3, \dots, x_n)$$

$$\stackrel{2}{\rightarrow} (\operatorname{Par}_n(x), \operatorname{Par}_n(\operatorname{Par}_n(x), x_2, \dots, x_n), x_3, \dots, x_n)$$

$$= (\operatorname{Par}_n(x), x_1, x_3, \dots, x_n)$$

$$\vdots$$

$$\stackrel{n}{\rightarrow} (\operatorname{Par}_n(x), x_1, x_2, \dots, x_{n-1}),$$

where $\stackrel{i}{\mapsto}$ denotes the update of state x_i .

In light of the above we obtain the commutative diagram

$$\mathbb{F}_{2}^{n} \xrightarrow{[\operatorname{Par}_{K_{n}}, \operatorname{id}]} \mathbb{F}_{2}^{n} \qquad (11)$$

$$\downarrow^{\iota_{\operatorname{Par}_{n}}} \qquad \qquad \downarrow^{\operatorname{proj}}$$

$$\hat{\mathbb{F}}_{2}^{n} \xrightarrow{\sigma_{n+1}} \hat{\mathbb{F}}_{2}^{n},$$

where

$$\operatorname{proj}(x_{1}, \dots, x_{n}, x_{n+1}) = (x_{1}, \dots, x_{n}),$$

$$\iota_{\operatorname{Par}_{n}}(x_{1}, \dots, x_{n}) = (x_{1}, \dots, x_{n}, \operatorname{Par}_{n}(x_{1}, \dots, x_{n})),$$
(13)

$$\sigma_{n+1}(x_1, x_2, \dots, x_{n+1}) = (x_{n+1}, x_1, \dots, x_n). \tag{14}$$

Note that proj : $\hat{\mathbb{F}}_2^n \to \mathbb{F}_2^n$ and $\iota_{\operatorname{Par}_n}$: $\mathbb{F}_2^n \to \hat{\mathbb{F}}_2^n$ are inverses. Similarly we obtain $[\operatorname{Par}_{K_n},\operatorname{id}]^{(2)}(x)=(x_n,\operatorname{Par}_n(x),x_1,x_2,\ldots,x_{n-2})$ and in general $[\operatorname{Par}_{K_n},\operatorname{id}]^{(k)}=\operatorname{proj}\circ\sigma_{n+1}^k\circ\iota_{\operatorname{Par}_n}$ showing that the order of an orbit of $[\operatorname{Par}_{K_n},\operatorname{id}]$ is a divisor of n+1.

Along the same lines we can show that $[Par_{K_n}, \pi]$ and $[Par_{K_n}, id]$ are topologically conjugated systems. We omit the details.

Thus we have that the length of every orbit of $[Par_{K_{n+1}}, \pi]$ is a divisor of n+2. However, it is easy to see that the orbit containing the state $(1, 0, 0, \ldots, 0)$ always have length n+2. To be explicit we have for n=7

$$\begin{array}{ccc} (1000000) \longrightarrow (1100000) \longrightarrow (0110000) \longrightarrow (0011000) \\ & & & & & \downarrow \\ (0000001) \longleftarrow (0000011) \longleftarrow (0000110) \longleftarrow (0001100) \; . \end{array}$$

Thus we deduce that $[\mathbf{Par}_{Q_2^n}, \eta_{\phi}(\pi)]$ has a periodic orbit of length n+2, and we are done.

So to summarize, we have obtained information about the structure of periodic orbits of SDS over n-cubes from corresponding simpler SDS over K_{n+1} .

Example 4 For the 4-dimensional cube Q_2^4 we can construct two graphs Y_1 and Y_2 as shown in figure 5 that have Q_2^4 as a common covering. In this particular case it means that we can obtain information about SDS over Q_2^4 from the corresponding SDS over Y_1 or Y_2 . Note that an SDS over Q_2^4 has $2^{2^4} = 65536$ states while an SDS over Y_1 or Y_2 has $2^{2^3} = 256 = \sqrt{65536}$ states. The two reductions were created from the subgroups $\{0, (0111)\}$ and $\{0, (1111)\}$ of \mathbb{F}_2^4 .

Summary

In this paper we presented a new class of discrete dynamical systems, SDS, which consists of a dependency graph Y, a collection of Y-local functions and an update schedule. We then studied a reduction methodology for SDS which allowed us to investigate key phase space features of a given system in the phase space of a much smaller system. In general there will be several such smaller systems. We then analyze this situation in detail in case of SDS over n-cubes where we construct a variety of reduced systems arising from certain symmetries of the given dependency graph. In particular we show under which conditions the complete graph K_{n+1} contains essential phase space information.

This is related to implementing computationally efficient simulations in the following way: Typically, in a simulation the system only realizes a small fraction of the total number of possible state configurations, that is, the representative trajectories only visit a small part of the phase space. Thus we see that the representative or important dynamics of the simulation quite possibly could have been realized by a much smaller and simpler simulation system. This is the role of the reduced system.

The development of SDS in its current state provides both a common conceptual base for a systematic investigation of simulation as well as a suite of mathematical results.

References

- [1] H. S. Mortveit and C. M. Reidys. Discrete, sequential dynamical systems. *Discrete Mathematics*, 226:281–295, 2001.
- [2] C. L. Barrett and C. M. Reidys. Elements of a theory of simulation I: Sequential CA over random graphs. *Appl. Math. and Comput.*, 98:241–259, 1999.
- [3] C. L. Barrett, H. S. Mortveit, and C. M. Reidys. Elements of a theory of simulation III: Equivalence of SDS. *Appl. Math. and Comput.*, 2000. In press.
- [4] C. L. Barrett, H. S. Mortveit, and C. M. Reidys. Elements of a theory of simulation IV: Fixed points, invertibility and equivalence. *Appl. Math. and Comput.*, 2000. submitted.
- [5] C. L. Barrett, H. S. Mortveit, and C. M. Reidys. Elements of a theory of simulation V: Phase space properties of sequential dynamical systems. *Appl. Math. and Comput.*, 2001. in progress.
- [6] C. M. Reidys. On Acyclic Orientations and SDS. *Adv. in Appl. Math.*, 2000. accepted.
- [7] C. M. Reidys. Acyclic Orientations of Random Graphs. *Adv. Appl. Math.*, 21:181–192, 1998.
- [8] C. M. Reidys. Phase space properties of SDS. *Adv. in Appl. Math.*, 2001. in progress.
- [9] C. L. Barrett, H. B. Hunt III, M. V. Marathe, S. S. Ravi, D. J. Rosenkrantz, and R. E. Stearns. Computational aspects of sequential dynamical systems I: Phase space properties. 2000. in preparation.

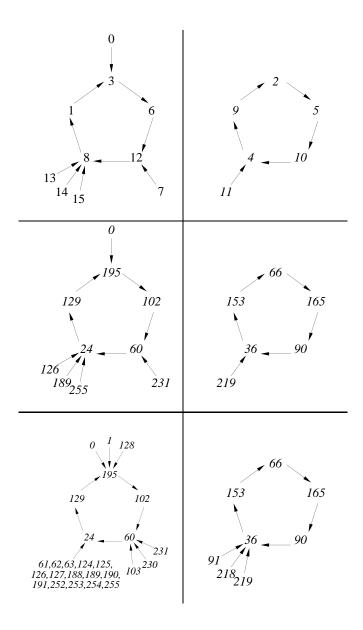


Figure 3. The top row shows the two five-cycles in $[\mathbf{Min}_{K_4}, \mathrm{id}]$. The second row shows the images of the top cycles under χ_{ϕ} , and the last row shows the corresponding periodic cycles in the digraph $\Gamma[\mathbf{Min}_{Q_2^3}, \eta_{\phi}(\mathrm{id}_4)]$. Note that we have encoded binary n-tuples as decimal numbers according to (8).

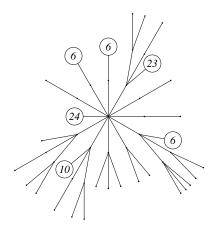


Figure 4. The structure of the components in $\Gamma[\mathbf{Min}_{Q_2^3},\eta_\phi(\mathrm{id}_4)]$ containing a fixed point. A single filled circle depicts a single state, while a circled number i depicts that there are i direct predecessors that do not have any predecessors themselves.

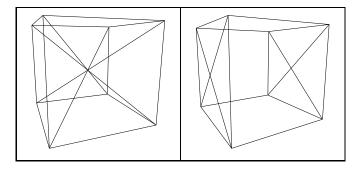


Figure 5. The only graphs up to isomorphism on 8 vertices of the form $H \setminus Q_2^4$.